Lefschetz-thimble path integral & its applications to real-time quantum tunneling

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Self-introduction

Current position: PhD student @ The University of Tokyo, JSPS fellow

Period this stay to UIC: June 02 - December 10

Group photo of Tetsuo Hatsuda's lab (RIKEN):

Research interest: Real-time dynamics (NEW!), Nonperturbative QFT (FRG), Superfluidity & Superconductivity, Ultracold atoms, Gauge theory.

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Introduction

Motivation

Real-time development of quantum systems gather much attentions:

- Nuclear physics (fusion, fission, ...)
- Quark-Gluon Plasma (thermalization, hydrodynamic description, ...)
- Quantum transport (Quantum dots, ultracold atoms, ...)

Importance of real-time correlators: Example

Real-time dynamics with small external perturbations
= Kinematics + Transport coefficient Linear response requires real-time correlators (Green-Kubo formula):

$$\text{viscosity, conductivity, ...} = \frac{V}{k_B T} \int_0^\infty \mathrm{d}t \underline{\langle J(t) J(0) \rangle}.$$

Real-time path integral

Description of real-time quantum dynamics needs for matrix elements of time-development operator $U(t_f, t_i) = \exp -\mathrm{i}H(t_f - t_i)/\hbar$:

$$K(x_f, t_f; x_i, t_i) = \int \mathcal{D}x \exp \mathrm{i}S[x(t)]/\hbar.$$

However,

- Real-time path integral is ill-defined
- Severe sign problem forbids us quantum Monte Carlo simulations.

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Question

Can we give an alternative to calculate strongly-coupled real-time dynamics?

Purpose of this talk

- Provide a basic framework to rewrite a path integral into a "'suitable" form
  $\Rightarrow$ Lefschetz-thimble path integral (E.Witten, arXiv:1001.2933)

$$\int \mathcal{D}x \exp iS[x]/\hbar = \sum_{\sigma} n_{\sigma} \int_{\mathcal{J}_{\sigma}} \mathcal{D}z \exp iS[z]/\hbar.$$

  $\Rightarrow$ Many research projects are now starting based on this formula:

  (finite-density QCD [Cristoforetti, Mulherjee, Scorzato, Renzo (2012-)],...,
  Resurgent transseries [Cherman, Dorigoni, Unsal (2014)],..., etc.)

- Application to quantum tunneling (Y.T., T. Koike, arXiv:1406:xxxx)

Lefschetz-thimble path integral

Real-time path integral and sign problems

Transition amplitude:

$$\langle \psi_f | \exp(-\mathrm{i}H(t_f - t_i)/\hbar) | \psi_i \rangle = \int \mathcal{D}x \, \overline{\psi_f(x_f)} \psi_i(x_i) \exp \mathrm{i}S[x]/\hbar$$

This is an oscillatory integral without any suppressions:

$$\left|\left| \exp(\mathrm{i}S/\hbar) \right|\right| = 1.$$

$\Rightarrow$ Real-time path integral is ill-defined.
$\Rightarrow$ Its quantum Monte Carlo simulation suffer from sign problem.

Zero-dimensional analogue of real-time path integrals

Airy function:

$$\mathrm{Ai}(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x \exp \mathrm{i} \left(\frac{x^3}{3} + \lambda x \right).$$

Common features of this Airy integral and real-time path integral:

- Both of them are ill-defined as Lebesgue integrations.
- With appropriate limits, they become finite due to oscillations.

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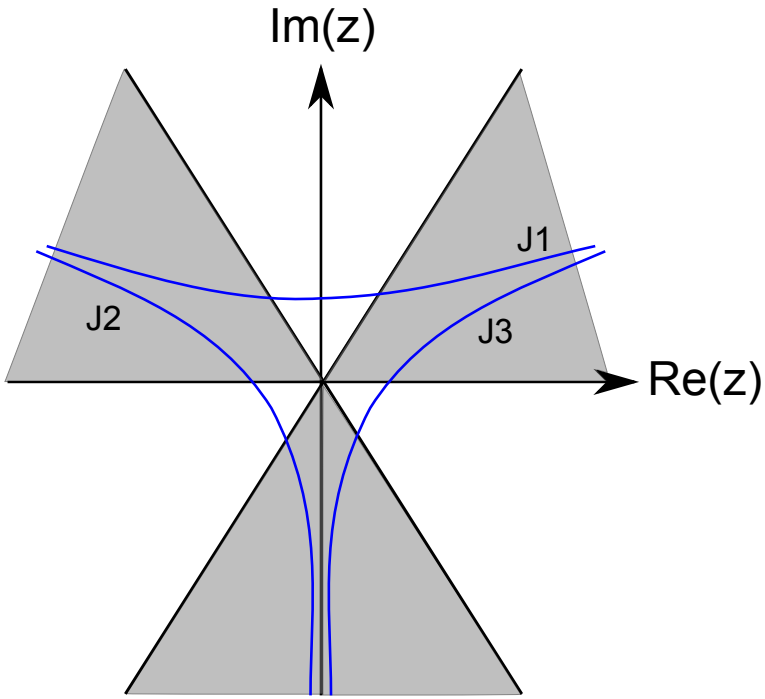
  1. Airy integral:

$$\mathrm{Ai}(\lambda) = \lim_{\varepsilon \to +0} \frac{1}{2\pi} \int \mathrm{d}x \exp(\mathrm{i} - \varepsilon \mathrm{sgn}(x)) \left(\frac{x^3}{3} + \lambda x \right)$$

  2. Path integral: $\mathrm{i}\varepsilon$ prescription in perturbative series, or Wick rotation $t \to -e^{\mathrm{i}\varepsilon} t$.

Change of integration contours

Behavior of the integrand in the complex z plane: $\exp \mathrm{i}(z^3/3 + z)$.



Blue lines $\mathcal{J}_\sigma$ refer to nice integration contours with good convergence: $\exp \mathrm{i}(z^3/3 + \lambda z) \to 0$ along blue lines:

$$\mathrm{Ai}(\lambda) = \frac{1}{2\pi} \int_{\mathcal{J}_1} \mathrm{d}z \exp \mathrm{i}(z^3/3 + \lambda z) = \frac{1}{2\pi} \int_{\mathcal{J}_2 + \mathcal{J}_3} \mathrm{d}z \exp \mathrm{i}(z^3/3 + \lambda z).$$

Necessity for Morse theory

Example of Airy integral clarify the following procedures for good convergence:

1. Regard the exponent $\mathrm{i}S[x(t)]$ as a holomorphic function(al) of $z \in \mathbb{C}^{[t_i,t_f]}$.
2. Find integration cycles $\mathcal{J}_\sigma$ with nice convergence so that $\exp \mathrm{i}S/\hbar \to 0$.
3. Represent the original integral as $\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \mathcal{D}z \exp(\mathrm{i}S[z]/\hbar)$

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- How can we calculate n_σ?

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Important!

Complex Morse theory (Picard–Lefschetz theory) answers all the above questions!

(E.Witten, arXiv:1001.2933)

Morse's downward flow

$\mathcal{J}_\sigma$ are defined by Morse's downward flows: $\dfrac{\partial z(t;u)}{\partial u} = -\overline{\dfrac{\delta \mathrm{i}S[z(t;u)]}{\delta z(t;u)}}$.

Properties:

1. Along those flows, $\mathrm{Re}(\mathrm{i}S) \to -\infty$.

$$\begin{aligned}\frac{\partial}{\partial u}\mathrm{Re}(\mathrm{i}S[z(t;u)]) &= \frac{1}{2}\int \mathrm{d}t \left(\frac{\delta \mathrm{i}S[z(t;u)]}{\delta z(t;u)}\frac{\partial z(t;u)}{\partial u} + \text{c.c.}\right) \\ &= -\int \mathrm{d}t \left|\frac{\delta \mathrm{i}S[z(t;u)]}{\delta z(t;u)}\right|^2 .\end{aligned}$$

2. Imaginary part is conserved along the flow:

$$\frac{\partial}{\partial u}\mathrm{Im}(\mathrm{i}S[z(t;u)]) = \frac{1}{2\mathrm{i}}\int \mathrm{d}t \left(\frac{\delta \mathrm{i}S[z(t;u)]}{\delta z(t;u)}\frac{\partial z(t;u)}{\partial u} - \text{c.c.}\right) = 0.$$

Lefschetz-thimble path integral

(E.Witten, arXiv:1001.2933, arXiv:1009.6032)

1. Solve the classical equation of motion, $\delta S[z] = 0$, in $\mathcal{X} = \{z : [t_i, t_f] \to \mathbb{C}\}$. Those solutions are denoted by z_σ with a label $\sigma \in \Sigma$.

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3. With some integers n_σ, rewrite the original path integral as

$$K(x_f, t_f; x_i, t_i) = \sum_{\sigma \in \Sigma} n_\sigma \int_{\mathcal{J}_\sigma} \mathcal{D}z \exp \mathrm{i} S[z]/\hbar.$$

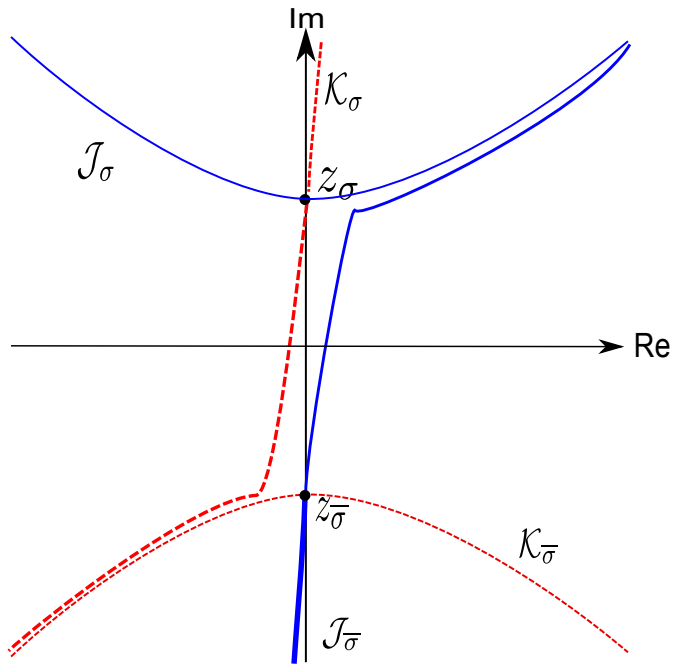
($n_\sigma = \langle \{x : [t_i, t_f] \to \mathbb{R}\}, \mathcal{K}_\sigma \rangle$, $\mathcal{K}_\sigma$: dual of $\mathcal{J}_\sigma$ defined by upward flows).

Example: Airy integral

Exponent: $\mathrm{i}S(z) = \mathrm{i}e^{\mathrm{i}0^+}(z^3/3 + z)$. Classical equation of motion:

$$\frac{\partial \mathrm{i}S(z)}{\partial z} = \mathrm{i}(z^2 + 1) = 0$$

Complex classical solutions: $z = \pm\mathrm{i}$.



Intersection numbers: $\langle \mathbb{R}, \mathcal{K}_\sigma \rangle = 1$, $\langle \mathbb{R}, \mathcal{K}_{\bar{\sigma}} \rangle = 0$.

Example: Airy integral

The Airy integral can now be written as

$$\mathrm{Ai}(+1) = \frac{1}{2\pi}\int_{\mathcal{J}_\sigma} \mathrm{d}z \exp \mathrm{i}(z^3/3 + z).$$

Summary on Airy integral:

1. S'(z)=0 has two complex solutions. $\Rightarrow$ There are two Lefschetz thimbles.
2. We can construct two independent convergent integrations:

$$\frac{1}{2\pi}\int_{\mathcal{J}_1} \mathrm{d}z \exp \mathrm{i}(z^3/3 + \lambda z), \quad \frac{1}{2\pi}\int_{\mathcal{J}_2} \mathrm{d}z \exp \mathrm{i}(z^3/3 + \lambda z)$$

(Recall that Airy equation $y'' + \lambda y = 0$ has two solutions.)

Quantum tunneling by Lefschetz-thimble path integral

Double-well potential

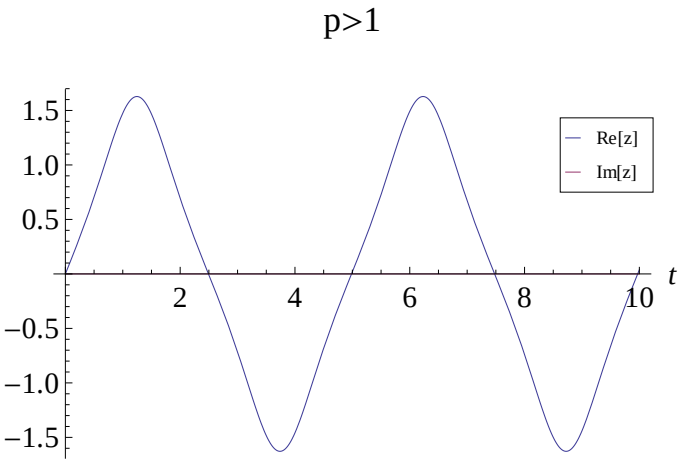
Classical action:

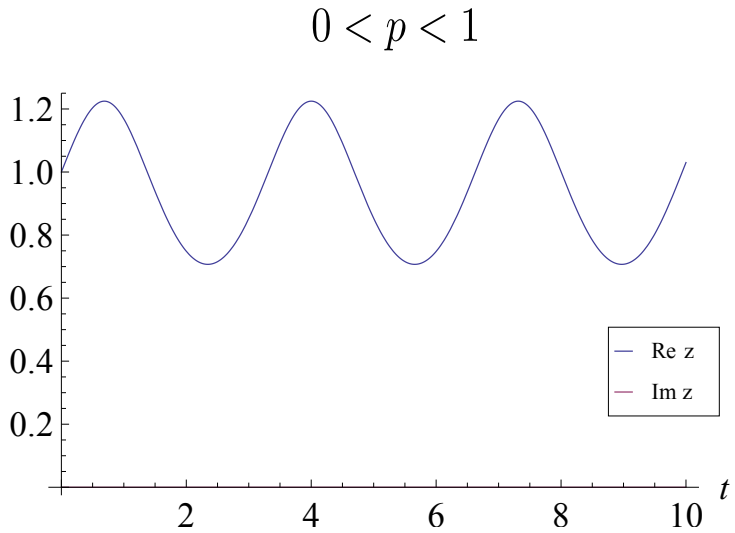
$$\mathrm{i}S[z] = \mathrm{i}\int \mathrm{d}t \left[\frac{1}{2}\dot{z}^2 - \frac{1}{2}(z^2-1)^2\right]$$

Energy conservation:

$$\frac{1}{2}\dot{z}^2 + \frac{1}{2}(z^2-1)^2 = \frac{1}{2}p^2$$

Real classical solutions:





Quantum tunneling & Symmetry restoration

Classical minima: $z = \pm 1$. $\Rightarrow$ Parity symmetry is not respected.

$\psi_\pm(x)$: localized state around two classical minima $x = \pm 1$.

Quantum oscillation:

$$|\langle \psi_+ | \exp -\mathrm{i}Ht/\hbar | \psi_- \rangle|^2 = \cos(\Delta E t/\hbar),$$

with

$$\Delta E \sim \exp -S_0/\hbar.$$

$\Rightarrow$ Ground state ψ_0 is parity even.

Question

Can we provide semi-classical description of quantum tunneling directly from real-time path integral?

Complex classical solutions

Let us find all the complex solutions of

$$\frac{\mathrm{d}^2 z}{\mathrm{d}t^2} = -2z(z^2-1).$$

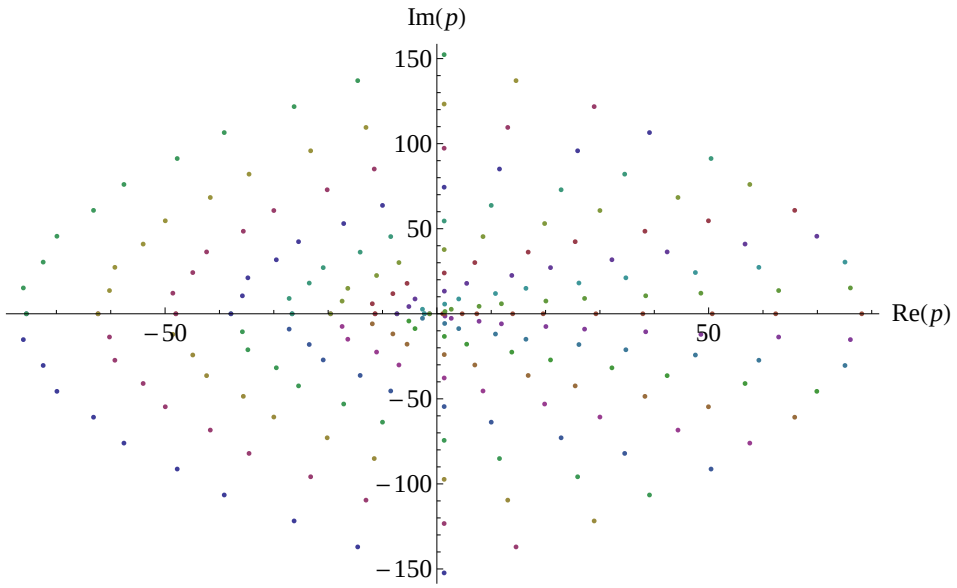
Analytic solution with $z(t_i) = x_i$:

$$z(t) = \sqrt{\frac{p^2-1}{2p}}\mathrm{sd}\left(\sqrt{2p}t + \mathrm{sd}^{-1}\left(\sqrt{\frac{2p}{p^2-1}}x_i, \sqrt{\frac{1+p}{2p}}\right), \sqrt{\frac{1+p}{2p}}\right).$$

$p^2/2$: Energy of the classical solution.
p is a complex parameter so that $z(t_f) = x_f$.

List of complex classical solutions

List of possible parameters p: (Y. T., T. Koike, arXiv:1406:xxxx)



Jacobian elliptic function has two half-periodicities:
$\mathrm{sd}(z+2K) = \mathrm{sd}(z+2\mathrm{i}K') = -sd(z)$. ($K$, K' : complete elliptic integrals)

The list of parameters p can be obtained as $(n, m \in \mathbb{Z})$

$$n\frac{K(\sqrt{(p+1)/2p})}{\sqrt{2p}} + m\frac{\mathrm{i}K(\sqrt{(p-1)/2p})}{\sqrt{2p}} = \frac{t_f - t_i}{2} + (\text{boundary terms}).$$

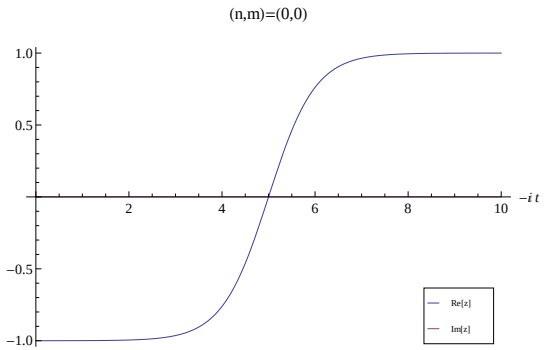
Imaginary-time instantons $\Rightarrow$ Sphalerons

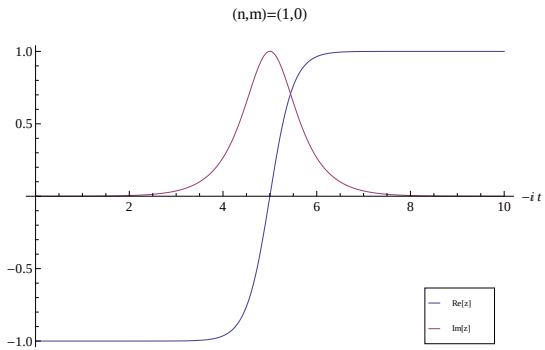
We obtained infinitely many complex solutions.

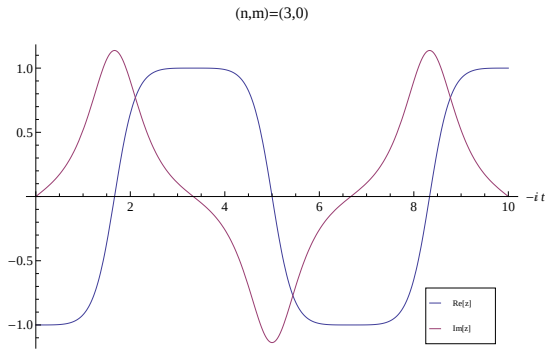
Question: Which describes real-time quantum tunneling?

Try analytic continuation of imaginary-time instantons to real-time processes.

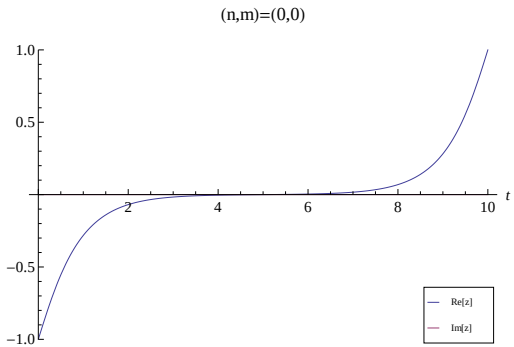
Imaginary-time processes:

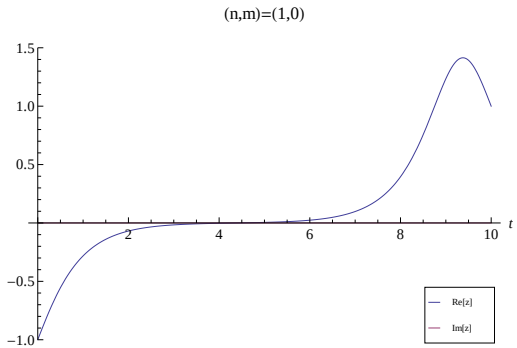


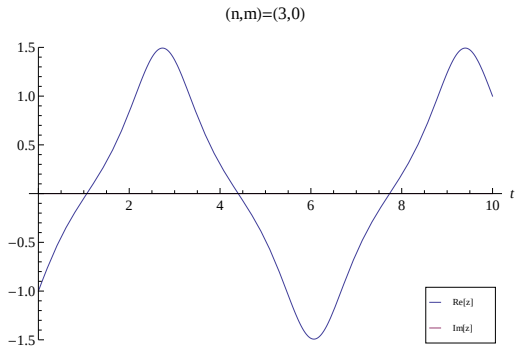




Real-time processes:

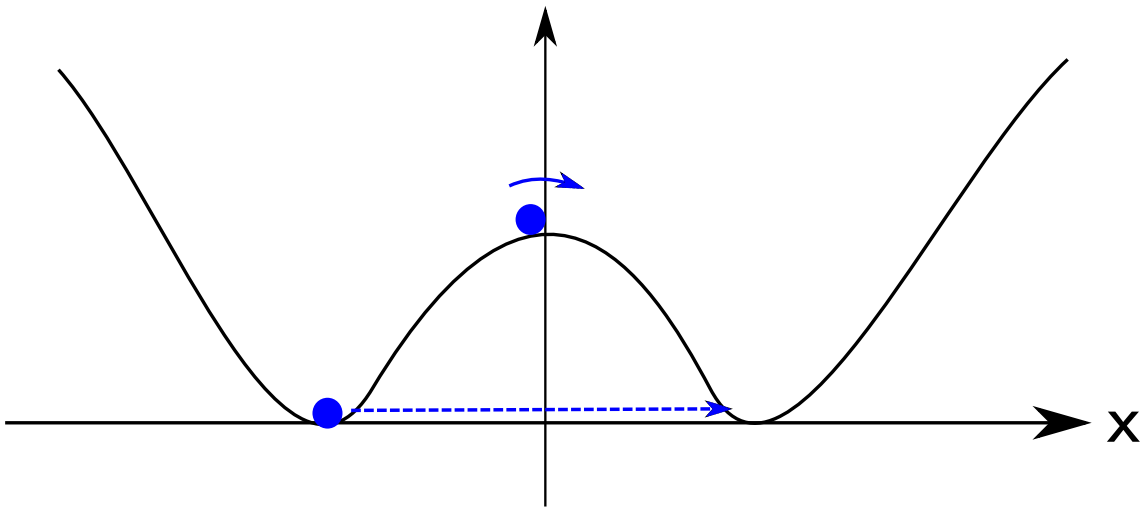






Do sphalerons describe symmetry restoration?

- Sphalerons has sufficient energies to overcome potential barrier classically.
  $\Rightarrow$ They are not suppressed in the semiclassical limit $\hbar \to 0$.
  (Klinkhamer, Manton (1984), Arnold, McLerran (1987))
- Quantum tunneling process does not have such large energies.



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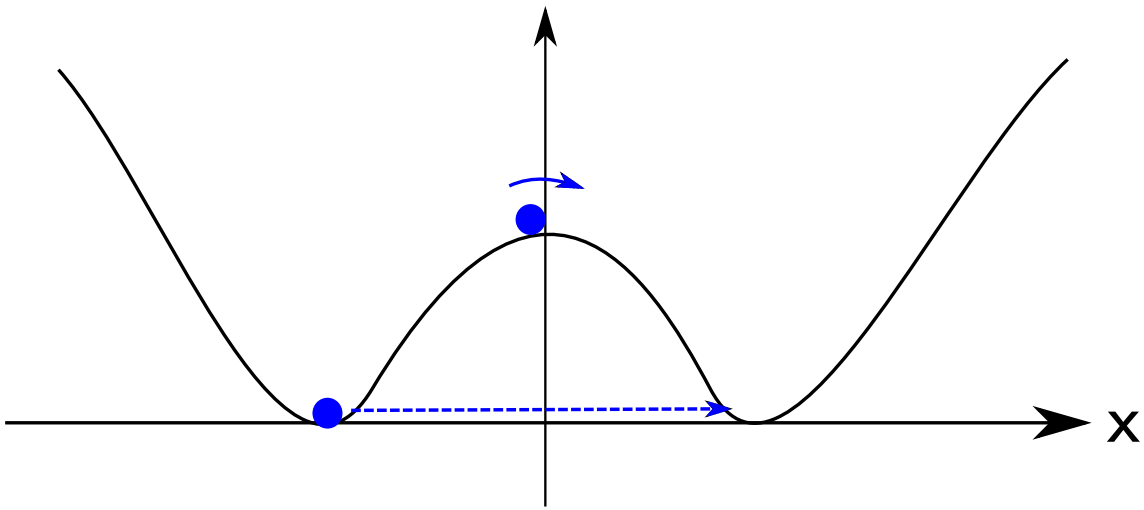
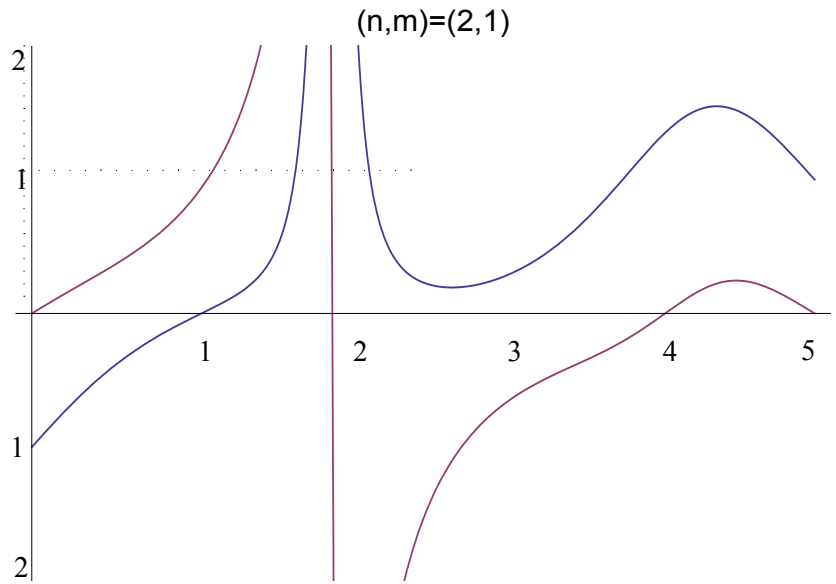


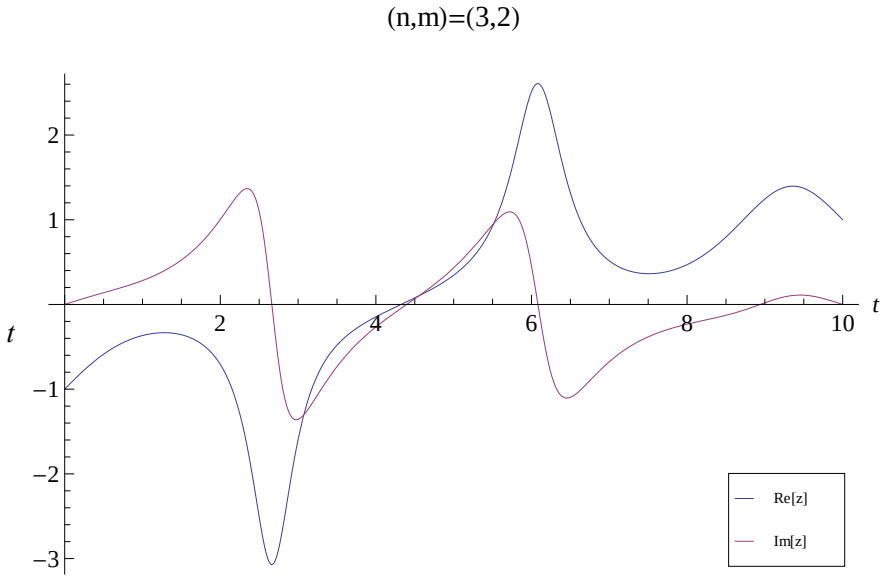
Important!

There must be another processes describing real-time tunneling.
They must satisfy $\mathrm{Re}(\mathrm{i}S) < 0$ *and* $n_\sigma \neq 0$.

Real-time tunneling = Complex classical solutions

There are many complex classical solutions with $\mathrm{Re}(\mathrm{i}S) < 0$:





Amplitudes of these processes behaves as $\exp(-|Re(\mathrm{i}S)|/\hbar)$ as $\hbar \to +0$.

Discussion

- We obtained a new understanding on quantum tunneling by exact semi-classical analysis of real-time path integral.
- Complex classical solutions are identified completely, and some of them show consistent behavior for quantum tunneling.
- Do they really have nonzero n_σ? Some of them must have, but how can we prove it?

Summary & Perspectives

Summary

- Lefschetz-thimble path integral may solve the sign problem, and then has wide applications to strongly-coupled systems.
- Exact semi-classical description of quantum tunneling is considered;
  1. Complex classical solutions are all determined.
  2. Real-time interpretation of imaginary-time instantons is obtained by analytic continuation. They are sphalerons.
  3. Real-time tunneling must be described by complex solutions with $\mathrm{Re}(\mathrm{i}S) < 0$.

Perspectives (& Open Problems)

- How can we calculate intersection numbers n_σ?
- Application to real-time dynamics of QCD.
  1. Sphaleron rate may become calculable. Time-dependence of μ_5 in anomalous hydro. then can be obtained!
- What is the relationship between Lefschetz-thimble path integral and complex Langevin equation.
  1. Both of them provides quantization of classical systems. Are they equivalent?
  2. Downward flow equation and stochastic equation have similar but different forms. What is the correspondence?